1-(4-methoxyphenyl)-2-phenylethanol 5422-47-9 | DTXSID60279078

5422-47-9	DTXSID60279078	

Model Performance

Model	Data
Widdel	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 79.4 °C

Global applicability domain: Inside

Local applicability domain index: 5.77e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

Image not found

Benzoin

Measured: 137 Predicted: 134 Image not found

Benzoin

Measured: 137 Predicted: 134

Image not found

Diphenylmethanol Measured: 69.0 Predicted: 75.5

Image not found

Cyclandelate
Measured: 56.0
Predicted: 57.5